C:\Program Files\Stnexp\Queries\563759dddd.str

chain nodes :
    15 16 19 20 27 44 45
ring nodes :
    1   2   3   4   5   6   7   8   9   10 11 12 13 14 28 29 30 31 32 33 34 35 36 37 38 39
    40 41
chain bonds :
    2-19 7-15 10-16 12-27 19-20 27-29 34-44 37-45
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13 13-14 28-29
    28-33 29-30 30-31 31-32 32-33 32-34 33-37 34-35 35-36 35-38 36-37 36-41 38-39
    39-40 40-41
exact/norm bonds :
    1-2 1-6 2-3 2-19 3-4 4-5 5-6 5-7 6-10 7-8 7-15 8-9 8-11 9-10 9-14 10-16 11-12
    12-13 12-27 13-14 19-20 27-29 34-44 37-45
normalized bonds :
    28-29 28-33 29-30 30-31 31-32 32-33 32-34 33-37 34-35 35-36 35-38 36-37 36-41
    38-39 39-40 40-41

G1:Br,F,I,CH3,Et,n-Pr,s-Bu,CF2,CN,C,S,Si

G2:C,N

G3:C,I,F,NO2,S,N,Si,OH,SH,MeO,EtO

Match level :
    1:Atom   2:Atom   3:CLASS   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
    12:Atom   13:Atom   14:Atom   15:CLASS   16:CLASS   19:CLASS   20:CLASS   27:CLASS   28:CLASS   29:CLASS
    30:CLASS   31:Atom   32:Atom   33:Atom   34:Atom   35:Atom   36:Atom   37:Atom   38:Atom   39:Atom
    40:Atom   41:Atom   44:CLASS   45:CLASS